

Multi-layer $S = \frac{1}{2}$ Heisenberg antiferromagnet

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Abstract

The multi-layer $S = \frac{1}{2}$ square lattice Heisenberg antiferromagnet with up to 6 layers is studied via various series expansions. For the systems with an odd number of coupled planes, the ground-state energy, staggered magnetization, and triplet excitation spectra are calculated via two different Ising expansions. The systems are found to have long range Néel order and gapless excitations for all ratios of interlayer to intralayer couplings, as for the single-layer system. For the systems with an even number of coupled planes, there is a second order transition point separating the gapless Néel phase and gapped quantum disordered spin liquid phase, and the critical points are located via expansions in the interlayer exchange coupling. This transition point is found to vary about inversely as the number of layers. The triplet excitation spectra are also computed, and at the critical point the normalized spectra appear to follow a universal function, independent of number of layers.

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I. INTRODUCTION

Low-dimensional quantum antiferromagnets exhibit many remarkable properties, and the study of these systems has been the subject of intense theoretical and experimental research in recent years. It is by now well established that one-dimensional Heisenberg antiferromagnets with integer spin have a gap in the excitation spectrum, whereas those with half-integer spin have gapless excitations. The former have a finite correlation length, while for the latter it is infinite with the spin-spin correlation function decaying to zero as a power law. In 2-dimensions, the unfrustrated square-lattice Heisenberg model has long range Néel order in the ground state. It has gapless Goldstone modes as expected. For the 3-dimensional Heisenberg model, one expects a stronger long-range Néel order [1] in the ground state.

In recent years much interest has focussed on systems with intermediate dimensionality and on questions of crossovers between $d = 1$ and $d = 2$. The investigations [2] showed that the crossover from the single Heisenberg chain to the two-dimensional antiferromagnetic square lattice, obtained by assembling chains to form a “ladder” of increasing width, is far from smooth. Heisenberg ladders with an even number of legs (chains) show a completely different behavior from odd-leg-ladders. While even-leg-ladders have a spin gap and short range correlations, odd-leg-ladders have no gap and power-law correlations.

What happens to the crossover from the two-dimensional antiferromagnetic square lattice to the three-dimensional antiferromagnetic simple cubic lattice, obtained by assembling planes to form a multi-layer system? The spin- S bilayer Heisenberg antiferromagnet has been well studied, and it has a second order transition [3,4] separating the Néel phase and dimer phase, and this critical points can be remarkably well fitted by the following linear relation:

$$(J_2/J_1)_c \simeq 3.72[S(S+1) - 0.068] . \quad (1)$$

The systems with more than two planes have not been studied, as far as we are aware. As in the case with even and odd numbers of coupled chains, we may expect the Heisenberg antiferromagnet on an odd number of coupled planes to show a fundamentally different behavior from that for an even number of coupled planes. The multilayer Heisenberg antiferromagnet has recently attracted attention also due to its relevance to the understanding of the magnetic properties of cuprate superconductors (such as $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$) containing two or more weakly coupled CuO_2 layers [5–7].

In this paper, we study the zero temperature properties of the n -layer, $S = \frac{1}{2}$, square lattice Heisenberg antiferromagnet, where each layer is composed of a nearest-neighbor Heisenberg model on a square lattice, and there is a further antiferromagnetic coupling between corresponding sites of each layer. The system can be described by the following Hamiltonian:

$$H = J_1 H_{\text{plane}} + J_2 H_{\text{rung}} \quad (2)$$

where

$$H_{\text{plane}} = \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} \mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha,j} \quad (3)$$

$$H_{\text{rung}} = \sum_i \sum_{\alpha=1}^{n-1} \mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha+1,i}$$

$\mathbf{S}_{\alpha,i}$ is a $S=1/2$ spin operator at site i of the α th layer, and $\langle i, j \rangle$ denotes a pair of nearest neighbor sites on a square lattice. Here J_1 is the interaction between nearest neighbor spins in one plane, and J_2 is the interaction between adjacent spins from different layers. We denote the ratio of couplings as y , that is, $y = J_2/J_1$. In the present paper, we study only the case of antiferromagnetic coupling, that is, both J_1 and J_2 are positive. In the small J_2/J_1 limit, the model describes n weakly interacting 2D Heisenberg antiferromagnets, where each of them is Néel ordered and possesses gapless Goldstone excitations. While in the large J_2/J_1 limit, the system reduces to weakly coupled rungs, and each rung is described by the Hamiltonian

$$h_{\text{rung}} = \sum_{\alpha=1}^{n-1} \mathbf{S}_{\alpha} \cdot \mathbf{S}_{\alpha+1} . \quad (4)$$

The ground state of h_{rung} is an $S = 0$ singlet for even n , or an $S = 1/2$ doublet for odd n . This implies that there are some fundamental differences between even and odd numbers of coupled planes. For an odd number of layers, the system can be mapped to the well-known single layer Heisenberg antiferromagnet at the large J_2 limit, and so the system should have Néel order for all ratios of interlayer to intralayer couplings. For an even number of layers, on the other hand, the system has a definite gap at the large J_2 limit, so we expect there is a transition separating the gapless Néel phase and gapped quantum disordered spin liquid phase at a certain critical ratio of J_2/J_1 , and this transition should lie in the universality class of the classical $d = 3$ Heisenberg model, as for the bilayer system [4].

To confirm the above arguments, we study these systems with up to 6 layers via various series expansions. This paper is organized as follows. In Section II, we develop two different Ising expansions for the 3 and 5-layer systems. The first one is the usual naive Ising expansion where we take the z -component of the Hamiltonian as the unperturbed Hamiltonian, and the rest of it as the perturbation. In the second Ising expansion, we choose the eigenstates of h_{rung} , which has an $S = 1/2$ doublet as the ground state, as the basis states. At the large J_2 limit, H_{plane} can be mapped to the well known spin- $\frac{1}{2}$ single layer Heisenberg antiferromagnet described by an effective Hamiltonian H_{eff} , so we can take H_{rung} and the z -component of H_{eff} as the unperturbed Hamiltonian, and the rest as the perturbation. The first Ising expansion works best in the small J_2/J_1 region, while the second one works best in the large J_2/J_1 region. Series are calculated for the ground-state energy, staggered magnetization, and triplet excitation spectra. Extrapolating these series to the isotropic limit, we find the system has long range Néel order and gapless excitation for all ratios of interlayer to intralayer couplings, as for the square lattice. In Section III, the 4 and 6-layer systems are studied by means of expansion in the interlayer coupling J_2 , and the transition points are located. The last section is devoted to a summary.

II. SYSTEM WITH ODD NUMBER OF COUPLED PLANES

For $n = 3$, the eigenstates for h_{rung} consist of

1) one $S_{\text{tot}} = 1/2$ doublet with energy $E_0^{\text{rung}} = -1$ and eigenstates

$$\begin{aligned}
S_{\text{tot}}^z = -\frac{1}{2} : \quad |(\frac{1}{2}, -\frac{1}{2}, -1)\rangle &= \frac{1}{\sqrt{6}}(|\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle - 2|\downarrow\uparrow\downarrow\rangle) \\
S_{\text{tot}}^z = \frac{1}{2} : \quad |(\frac{1}{2}, \frac{1}{2}, -1)\rangle &= \frac{1}{\sqrt{6}}(|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle - 2|\uparrow\downarrow\uparrow\rangle)
\end{aligned} \tag{5}$$

where the arrows represent, from left to right, the z -components of S_α ($\alpha = 1, 2, \dots, n$), and the eigen states are denoted by $(S_{\text{tot}}, S_{\text{tot}}^z, E)$. S_{tot} , S_{tot}^z and E are the total spin, the z -component of the total spin, and its corresponding eigenvalue, respectively. This is the ground state of h_{rung} .

2) another $S_{\text{tot}} = 1/2$ doublet with energy $E_1^{\text{rung}} = 0$ and eigenstates

$$\begin{aligned}
S_{\text{tot}}^z = -\frac{1}{2} : \quad |(\frac{1}{2}, -\frac{1}{2}, 0)\rangle &= \frac{1}{\sqrt{2}}(|\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\rangle) \\
S_{\text{tot}}^z = \frac{1}{2} : \quad |(\frac{1}{2}, \frac{1}{2}, 0)\rangle &= \frac{1}{\sqrt{2}}(|\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle)
\end{aligned} \tag{6}$$

3) one $S_{\text{tot}} = \frac{3}{2}$ quartet with energy $E_2^{\text{rung}} = 1/2$ and eigenstates

$$\begin{aligned}
S_{\text{tot}}^z = -\frac{3}{2} : \quad |(\frac{3}{2}, -\frac{3}{2}, \frac{1}{2})\rangle &= |\downarrow\downarrow\downarrow\rangle \\
S_{\text{tot}}^z = -\frac{1}{2} : \quad |(\frac{3}{2}, -\frac{1}{2}, \frac{1}{2})\rangle &= \frac{1}{\sqrt{3}}(|\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle) \\
S_{\text{tot}}^z = \frac{1}{2} : \quad |(\frac{3}{2}, \frac{1}{2}, \frac{1}{2})\rangle &= \frac{1}{\sqrt{3}}(|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle) \\
S_{\text{tot}}^z = \frac{3}{2} : \quad |(\frac{3}{2}, \frac{3}{2}, \frac{1}{2})\rangle &= |\uparrow\uparrow\uparrow\rangle
\end{aligned} \tag{7}$$

So in the limit of $J_1/J_2 = 0$, the ground state of the whole system is the direct product of the ground states of each rung, which are degenerate with $S = \frac{1}{2}$ and $S^z = \pm\frac{1}{2}$, and so it is 2^N -fold degenerate (N is no. of sites). A finite value of J_1 lifts this degeneracy (to 2). In this 2^N -dimensional subspace, one can define an effective Hamiltonian H_{eff} which includes all interactions H_{plane} . To first order in J_1/J_2 we obtain [8]

$$H_{\text{eff}} = J_{\text{eff}} \sum_{\langle ij \rangle} \mathbf{S}_i^{\text{eff}} \cdot \mathbf{S}_j^{\text{eff}} \tag{8}$$

with effective coupling

$$J_{\text{eff}} = J_1 \tag{9}$$

Note that J_{eff} for Heisenberg ladder systems has been computed by N. Hatano and Y. Nishiyama [8], and their results can also be applied to the multi-plane Heisenberg antiferromagnet discussed here.

Therefore the ground state energy per site to first order in J_1/J_2 will be

$$E_0/N = (J_2 E_0^{\text{rung}} + E_0^{\text{sq}} J_{\text{eff}})/n \quad (10)$$

where $E_0^{\text{sq}} = -0.6693$ is the ground state energy per site for the square lattice [9].

To find out the staggered magnetization at large J_2 limit, one needs to look at the results of the operator $S_1^z - S_2^z + S_3^z$ on the states $|(\frac{1}{2}, -\frac{1}{2}, -1)\rangle$ and $|(\frac{1}{2}, \frac{1}{2}, -1)\rangle$:

$$\begin{aligned} (S_1^z - S_2^z + S_3^z)|(\frac{1}{2}, -\frac{1}{2}, -1)\rangle &= -\frac{5}{6}|(\frac{1}{2}, -\frac{1}{2}, -1)\rangle + 0.942809|(\frac{3}{2}, -\frac{1}{2}, \frac{1}{2})\rangle \\ (S_1^z - S_2^z + S_3^z)|(\frac{1}{2}, \frac{1}{2}, -1)\rangle &= \frac{5}{6}|(\frac{1}{2}, \frac{1}{2}, -1)\rangle - 0.942809|(\frac{3}{2}, \frac{1}{2}, \frac{1}{2})\rangle \end{aligned} \quad (11)$$

If we only keep the states which are the ground states of h_{rung} , and compare the above relations with that for the single layer square lattice, we can get the staggered magnetization at the large J_2 limit as

$$M \equiv \frac{1}{N} \sum_{i,\alpha} \langle (-1)^{i+\alpha} S_{i,\alpha}^z \rangle_0 = \frac{5M^{\text{sq}}}{3n} = 0.1706(6) \quad (12)$$

where $M^{\text{sq}} = 0.307(1)$ is the staggered magnetization for the single layer square lattice. [9]

For other odd n values, the ground states of h_{rung} are also two spin- $\frac{1}{2}$ doublet states. In Table I, we listed the ground state energy E_0^{rung} of h_{rung} , the effective coupling J_{eff} and the staggered magnetization M at the large J_2 limit for $n = 3, 5, 7, 9, 11$, and these are also shown in Figure 1, where we can see that as n increases, J_{eff}/J_1 is generally close to unity but increases monotonically, while M/M^{sq} decreases about as $n^{-1/2}$. At the limit of $n \rightarrow \infty$, we expect that J_{eff}/J_1 approaches a constant [8], while M/M^{sq} decreases to zero.

Since at both large and small y limits, the system can be reduced to a single plane Heisenberg antiferromagnet, we expect that unlike the bilayer Heisenberg antiferromagnets, there is no transition at any value of y .

To study the properties of these systems, we develop following two different Ising expansions.

The first one is the usual naive Ising expansion where we take the z -component of the Hamiltonian as the unperturbed Hamiltonian H_0 , and the rest of it as the perturbation V : we write the Hamiltonian for the Heisenberg-Ising model as:

$$H/J_1 = H_0 + xV \quad (13)$$

where

$$\begin{aligned} H_0 &= \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} S_{\alpha,i}^z S_{\alpha,j}^z + y \sum_{\alpha=1}^{n-1} \sum_i S_{\alpha,i}^z S_{\alpha+1,i}^z + t \sum_{\alpha,i} \epsilon_{\alpha,i} S_{\alpha,i}^z \\ V &= \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} (S_{\alpha,i}^x S_{\alpha,j}^x + S_{\alpha,i}^y S_{\alpha,j}^y) + y \sum_{\alpha=1}^{n-1} \sum_i (S_{\alpha,i}^x S_{\alpha+1,i}^x + S_{\alpha,i}^y S_{\alpha+1,i}^y) - t \sum_{\alpha,i} \epsilon_{\alpha,i} S_{\alpha,i}^z \end{aligned} \quad (14)$$

and $\epsilon_{\alpha,i} = \pm 1$ on the two sublattices. The last term in both H_0 and V is a local staggered field term, which can be included to improve convergence. The limits $x = 0$ and $x = 1$ correspond to the Ising model and the isotropic Heisenberg model respectively. The operator H_0 is taken as the unperturbed Hamiltonian, with the unperturbed ground state being the usual Néel state. The operator V is treated as a perturbation. It flips a pair of spins on neighbouring sites. The linked-cluster expansion method has been previously reviewed in several articles [10–12], and will not be repeated here.

The Ising series have been calculated for the ground state energy per site E_0/N , the staggered magnetization M , and the lowest lying triplet excitation spectrum $\Delta(k_x, k_y)$ for several ratios of couplings and (simultaneously) for several values of t up to order x^{11} for $n = 3$ or order x^9 for $n = 5$. The triplet excitation spectrum is computed for $n = 3$ only. The resulting series for E_0/N and M for $y = 0.5, 1, 2$ are listed in Tables II, and the other series are available on request.

There are three bands of the spin-wave dispersion for 3-layer systems. In the Ising limit, 2 bands have initial excitations located in the side planes, and the third band has it in the middle plane. From the series one can see that all three bands have the following symmetry:

$$\Delta(k_x, k_y) = \Delta(k_y, k_x) = \Delta(\pi - k_x, \pi - k_y) \quad (15)$$

Since at the large J_2 limit the system can be mapped to the well known spin- $\frac{1}{2}$ single layer Heisenberg antiferromagnet with effective Hamiltonian H_{eff} defined in Eq. (8), we can develop, in the basis of the eigenstates of h_{rung} , another Ising expansion, the so called “modified Ising expansion”, where we take H_{rung} and the z -component of H_{eff} as the unperturbed Hamiltonian, and the rest as the perturbation. That is, we write the Hamiltonian for the Heisenberg-Ising model as:

$$H = H'_0 + xV' \quad (16)$$

where

$$\begin{aligned} H'_0 &= J_2 H_{\text{rung}} + J_{\text{eff}} \sum_{\langle i,j \rangle} S_i^{\text{eff},z} S_j^{\text{eff},z} + t \sum_i \epsilon_i S_i^{\text{tot},z} \\ V' &= J_1 H_{\text{plane}} - J_{\text{eff}} \sum_{\langle i,j \rangle} S_i^{\text{eff},z} S_j^{\text{eff},z} - t \sum_i \epsilon_i S_i^{\text{tot},z} \end{aligned} \quad (17)$$

$S_i^{\text{tot},z}$ is z -component of the total spin for i th rung, and again the last term in both H'_0 and V' is a local staggered field term, which can be included to improve convergence. The limits $x = 0$ and $x = 1$ correspond to the Ising model and the isotropic Heisenberg model respectively. The operator H'_0 is taken as the unperturbed Hamiltonian, with the unperturbed ground state being the usual Néel state. The operator V' is treated as a perturbation. The detailed eigenvalues and eigenstates of h_{rung} and also the matrix elements V' under the eigenstates of h_{rung} for both $n = 3$ and $n = 5$ are available from the author.

Here the Ising series have been calculated for the ground state energy per site E_0/N , and the staggered magnetization M for several ratios of couplings and (simultaneously) for several values of t up to order x^6 for $n = 3$ or order x^4 for $n = 5$. The resulting series for

E_0/N and M for $y = 5, 10, 20$ are listed in Tables II, and the other series are available on request.

Having obtained the series for the above two Ising expansions we try to extrapolate the series to the isotropic point ($x = 1$). For this purpose, we first transform the series to a new variable

$$\delta = 1 - (1 - x)^{1/2} \quad (18)$$

to remove the singularity at $x = 1$ predicted by the spin-wave theory. This was first proposed by Huse [13] and was also used in our earlier work on the square lattice case [9]. We then use both integrated first-order inhomogeneous differential approximants [14] and naive Padé approximants to extrapolate the series to the isotropic point $\delta = 1$ ($x = 1$). The results for the ground state energy per site E_0/N , and the staggered magnetization M are shown in Figs. 2-3. The results for $J_2 = 0$ presented in the figures are taken from our earlier work on the single-layer square lattice [9], while the results for $J_1/J_2 = 0$ are taken from the mapping of the system on to the single layer system. The asymptotic behaviour, Eq. (10), of the ground state energy is also shown in Fig. 2 as dotted line, and they match on to those Ising expansions very well. The results from two Ising expansion also match each other very well in certain regions of coupling. We note that M first increases for small J_2/J_1 , passes through a maximum at about $J_2/J_1 \simeq 1$, and then decreases for larger values of J_2/J_1 . The reason that in the case of small J_2/J_1 , the interlayer coupling enhances the antiferromagnetic long-range order is that the system acquires a weak three dimensionality and quantum fluctuations are suppressed. The spin-wave theory for the bilayer Heisenberg antiferromagnet predicts that M should be proportional to $(J_2/J_1)^{1/2}$ in the small J_2/J_1 region, we can expect this will happen for any multi-layer system, and so in Figs. 2-3 we show E_0 and M as a function of $(J_2/J_1)^{1/2}/[(J_2/J_1)^{1/2} + 1]$ to exhibit this behaviour. From Fig. 3, we can see that in the small J_2/J_1 region, the 5-layer system has slightly stronger Néel order than the 3-layer system, while in the large J_2/J_1 region, the 3-layer system has stronger Néel order.

Figs. 4-6 show the three bands of triplet excitation spectra of the 3-layer system obtained from the naive Ising expansion. From these graphs, we can see that all of the dispersion relations have a minimum located at $(k_x, k_y) = (0, 0)$ (or (π, π) by symmetry), where two of these three bands have a definite gap as long as $J_2 \neq 0$, while the third (the outer symmetry band) is consistent with a gapless spectrum for all values of J_2 .

III. SYSTEM WITH EVEN NUMBER OF COUPLED PLANES

For even n , the ground state of h_{rung} is a $S = 0$ singlet. For example, the eigenstates of h_{rung} for $n = 4$ consist of

1) one $S_{\text{tot}} = 0$ singlet with energy $E_0^{\text{rung}} = (-3 - 2\sqrt{3})/4$ and eigenstate

$$|(0, 0, E_0^{\text{rung}})\rangle = c_1(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle) - c_2(|\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle) + c_3(|\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle) \quad (19)$$

where

$$c_1 = \frac{3 + 2\sqrt{3}}{6\sqrt{26 + 15\sqrt{3}}}, \quad c_2 = \frac{12 + 7\sqrt{3}}{6\sqrt{26 + 15\sqrt{3}}}, \quad c_3 = \frac{9 + 5\sqrt{3}}{6\sqrt{26 + 15\sqrt{3}}} \quad (20)$$

This is the ground state of H_{rung} .

2) one $S_{\text{tot}} = 1$ triplet with energy $E_1^{\text{rung}} = (-1 - 2\sqrt{2})/4$ and eigenstates

$$\begin{aligned} S_{\text{tot}}^z = -1 : \quad & |(1, -1, E_1^{\text{rung}})\rangle = c_4(|\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\downarrow\rangle) + c_5(|\downarrow\downarrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\downarrow\rangle) \\ S_{\text{tot}}^z = 0 : \quad & |(1, 0, E_1^{\text{rung}})\rangle = c_4(|\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle) + c_5(|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle) \\ S_{\text{tot}}^z = 1 : \quad & |(1, 1, E_1^{\text{rung}})\rangle = c_4(|\downarrow\uparrow\uparrow\uparrow\rangle - |\uparrow\uparrow\uparrow\downarrow\rangle) + c_5(|\uparrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle) \end{aligned} \quad (21)$$

where

$$c_4 = \frac{1 + \sqrt{2}}{2\sqrt{10 + 7\sqrt{2}}}, \quad c_5 = \frac{3 + 2\sqrt{2}}{2\sqrt{10 + 7\sqrt{2}}} \quad (22)$$

3) another $S_{\text{tot}} = 1$ triplet with energy $E_2^{\text{rung}} = -1/4$ and eigenstates:

$$\begin{aligned} S_{\text{tot}}^z = -1 : \quad & |(1, -1, E_2^{\text{rung}})\rangle = \frac{1}{2}(|\downarrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\downarrow\rangle - |\downarrow\downarrow\downarrow\downarrow\rangle) \\ S_{\text{tot}}^z = 0 : \quad & |(1, 0, E_2^{\text{rung}})\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle) \\ S_{\text{tot}}^z = 1 : \quad & |(1, 1, E_2^{\text{rung}})\rangle = \frac{1}{2}(|\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle) \end{aligned} \quad (23)$$

4) another $S_{\text{tot}} = 0$ singlet with energy $E_3^{\text{rung}} = (-3 + 2\sqrt{3})/4$ and eigenstate

$$|(0, 0, E_3^{\text{rung}})\rangle = c_2(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle) - c_1(|\downarrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle) - c_3(|\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle) \quad (24)$$

5) another $S_{\text{tot}} = 1$ triplet with energy $E_4^{\text{rung}} = (-1 + 2\sqrt{2})/4$ and eigenstates:

$$\begin{aligned} S_{\text{tot}}^z = -1 : \quad & |(1, -1, E_4^{\text{rung}})\rangle = c_5(|\downarrow\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\downarrow\rangle) + c_4(|\downarrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\downarrow\rangle) \\ S_{\text{tot}}^z = 0 : \quad & |(1, 0, E_4^{\text{rung}})\rangle = c_5(|\downarrow\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\downarrow\rangle) + c_4(|\downarrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\downarrow\rangle) \\ S_{\text{tot}}^z = 1 : \quad & |(1, 1, E_4^{\text{rung}})\rangle = c_5(|\downarrow\uparrow\uparrow\uparrow\rangle - |\uparrow\uparrow\uparrow\downarrow\rangle) + c_4(|\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle) \end{aligned} \quad (25)$$

6) one $S_{\text{tot}} = 2$ quintuplet with energy $E_5^{\text{rung}} = 3/4$ and eigenstates

$$\begin{aligned} S_{\text{tot}}^z = -2 : \quad & |(2, -2, E_5^{\text{rung}})\rangle = |\downarrow\downarrow\downarrow\downarrow\rangle \\ S_{\text{tot}}^z = -1 : \quad & |(2, -1, E_5^{\text{rung}})\rangle = \frac{1}{2}(|\downarrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\downarrow\rangle) \\ S_{\text{tot}}^z = 0 : \quad & |(2, 0, E_5^{\text{rung}})\rangle = \frac{1}{\sqrt{6}}(|\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle) \\ S_{\text{tot}}^z = 1 : \quad & |(2, 1, E_5^{\text{rung}})\rangle = \frac{1}{2}(|\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\rangle) \\ S_{\text{tot}}^z = 2 : \quad & |(2, 2, E_5^{\text{rung}})\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle \end{aligned} \quad (26)$$

So at the limit of $J_1/J_2 = 0$, the ground state of the whole system is the direct product of the ground state of each rung. Unlike the case for odd value of n , there is not degeneracy in this ground state, and the system has a definite excitation gap.

The operator $S_1^z - S_2^z + S_3^z - S_4^z$ on the ground state $|(0, 0, E_0^{\text{rung}})\rangle$ gives

$$(S_1^z - S_2^z + S_3^z - S_4^z)|(0, 0, E_0^{\text{rung}})\rangle = -1.45728|(1, 0, E_1^{\text{rung}})\rangle + 0.6036258|(1, 0, E_4^{\text{rung}})\rangle \quad (27)$$

Again unlike the case for odd n , the right hand side of the above equation does not contain the ground state $|(0, 0, E_0^{\text{rung}})\rangle$, so in the large J_2 limit, the staggered magnetization M is zero, that is, the system is in a quantum disordered spin liquid state. So we expect there is a transition separating the gapless Néel phase and gapped quantum disordered spin liquid phase at a certain critical ratio of J_2/J_1 , and we expect that this is true for any even number of layers.

To locate the transition point, we can develop the expansions around the large interlayer coupling limit, that is, we can construct an expansion in $1/y$ by treating the operator H_{rung} as the unperturbed Hamiltonian and operator H_{plane} as a perturbation. We have developed the expansion for the $T = 0$ ground state energy per site E_0/N , the antiferromagnetic susceptibility χ , and the lowest lying triplet excitation spectrum $\Delta(k_x, k_y)$ up to a certain order (see Table III) for $n = 4$ and 6 . The resulting power series in $1/y$ for E_0/N and χ are presented in Table III. The series for the minimum energy gap $m = \Delta(\pi, \pi)$ is also listed in Table III. The series for the excitations spectra $\Delta(k_x, k_y)$ are available on request.

To determine the critical point, we construct Dlog Padé approximants [14] to the χ and m series. Since the transition should lie in the universality class of the classical $d = 3$ Heisenberg model (our analysis also supports this), we expect that the critical index for χ and m should be approximately 1.40 and 0.71, respectively. The exponent-biased Dlog Padé approximants give the critical point $(J_1/J_2)_c = 0.213(5)$ for $n = 4$, and $(J_1/J_2)_c = 0.145(10)$ for $n = 6$. The critical points $(J_1/J_2)_c$ as function of $1/n$ are shown in Fig. 7 (the results for $n = 2$ are taken from a previous calculation [4]), where we can see they can be well fitted by $(J_1/J_2)_c = 0.913/n - 0.250/n^2$. So $(J_1/J_2)_c$ should be proportional to $1/n$ at the large n limit.

The triplet excitation spectra $\Delta(k_x, k_y)$ at the critical point for $n = 4, 6$ are illustrated in Fig. 8(a): the results for $n = 2$ are also displayed here for ease of comparison. We can see, as in the case of the bilayer Heisenberg antiferromagnet [4], the direct sum to the series is indeed consistent with the Padé approximants that one can construct. The spectra have their maximum value $\Delta(0, 0)$ at $(k_x, k_y) = (0, 0)$. In Fig. 8(b), we plot the function for $\Delta(k_x, k_y)/\Delta(0, 0)$ along high-symmetry cuts through the Brillouin zone, and we can see this function appears to be an universal function, independent of the number of layers n . We have no independent theory to explain it at present, but argue this may be due to the fact they belong to the same universality class.

IV. CONCLUSIONS

We have presented and analyzed various perturbation series expansions for multi-layer, $S = \frac{1}{2}$, square lattice Heisenberg model with up to 6 coupled planes. Like Heisenberg ladder system, the Heisenberg antiferromagnet on an odd number of coupled planes shows a fundamentally different behavior from that for an even number of coupled planes.

For an odd number of layers, the system can be mapped to the well-known single layer Heisenberg antiferromagnet at the large J_2 limit, and so the system should have Néel order for all ratios of interlayer to intralayer couplings: that is, it is similar to the case of the square lattice. The staggered magnetization M at the large J_2/J_1 limit is computed up to 11-layers, and we found M should decrease to zero as $n^{-1/2}$ in the large n limit. For the systems with 3 and 5-layers, two Ising expansions have been developed, and series are calculated for

the ground-state energy, the staggered magnetization, and the triplet excitation spectra. Extrapolating these series to the isotropic limit, we find the system has long range Néel order and gapless excitations for all ratios of interlayer to intralayer couplings.

For an even numbers of layers, expansions in the interlayer coupling have been developed for both 4 and 6 layers. The systems turn out to have a second order transition separating a gapless Néel phase and a gapped quantum disordered spin liquid phase, where the critical point is determined to be $(J_1/J_2)_c = 0.213(5)$ for $n = 4$, and $(J_1/J_2)_c = 0.145(10)$ for $n = 6$, and this critical point should be proportional to $1/n$ in the large n limit. The triplet excitation spectra are also computed, and at the critical point, it turns out that the excitation spectrum, after normalization by its maximum value, appears to be an universal function, independent of the number of layers. This may be due to the fact that they belong to the same universality class.

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FIGURES

FIG. 1. The effective coupling J_{eff} and the staggered Magnetization M for odd n at the limit $J_2/J_1 \rightarrow \infty$ as function of $n^{-1/2}$, and the solid line is the least square polynomial fit $M/M^{\text{sq}} = 1.125n^{-1/2} - 0.532n^{-1} + 0.431n^{-3/2}$.

FIG. 2. The rescaled ground-state energy per site E_0/N for 3 and 5-layers as function of $(J_2/J_1)^{1/2}/[(J_2/J_1)^{1/2} + 1]$. The solid (open) points with error bars are the estimates from the naive (modified) Ising expansions, and the dotted curve at large $(J_2/J_1)^{1/2}$ region is the asymptotic behaviour, i.e., Eq. (10).

FIG. 3. The staggered magnetization M for 3 and 5-layers *versus* $(J_2/J_1)^{1/2}/[(J_2/J_1)^{1/2} + 1]$. The solid (open) points with error bars are the estimates from the naive (modified) Ising expansions.

FIG. 4. Plot of symmetric spin-triplet excitation (in side planes) spectrum $\Delta(k_x, k_y)$ (derived from the naive Ising expansions) along high-symmetry cuts through the Brillouin zone for the three-layer system with coupling ratios $J_2/J_1 = 0, 0.5, 1$ (shown in the figure from the bottom to the top respectively).

FIG. 5. Plot of antisymmetric spin-triplet excitation (in side planes) spectrum $\Delta(k_x, k_y)$ (derived from the naive Ising expansions) along high-symmetry cuts through the Brillouin zone for the three-layer system with coupling ratios $J_2/J_1 = 0, 0.5, 1, 2, 4$ (shown in the figure from the bottom to the top respectively).

FIG. 6. Plot of spin-triplet excitation (in middle plane) spectrum $\Delta(k_x, k_y)$ (derived from the naive Ising expansions) along high-symmetry cuts through the Brillouin zone for the three-layer system with coupling ratios $J_2/J_1 = 0, 0.1, 0.25, 0.5, 1$ (shown in the figure from the bottom to the top respectively).

FIG. 7. Plot of the critical points $(J_1/J_2)_c$ *versus* $1/n$ for even number of coupled planes. The solid points with error bars are the estimates from expansions about interlayer coupling, and the solid line is the least square polynomial fit $(J_1/J_2)_c = 0.913/n - 0.250/n^2$.

FIG. 8. Plot of the triplet excitation spectrum $\Delta(k_x, k_y)$ (a) and spectrum after normalization by its maximum value (b) along high-symmetry cuts through the Brillouin zone for the $n = 2, 4, 6$ systems at the transition point, the lines are the estimates by direct sum to the dimer series, and the points are the estimates of the Padé approximants to the series.

TABLES

TABLE I. the ground state energy E_0^{rung} of h_{rung} , the effective coupling J_{eff} and the staggered magnetization M in the limit $J_2/J_1 \rightarrow \infty$ for odd n up to $n = 11$.

n	E_0^{rung}/n	J_{eff}/J_1	M/M^{sq}
3	-0.33333333	1	0.555556
5	-0.38557725	1.016938829	0.435575
7	-0.40517710	1.034391333	0.372626
9	-0.41514686	1.050406957	0.331978
11	-0.42109939	1.064819159	0.302836

TABLE II. Series coefficients of naive and modified Ising expansions of three layer system for the ground-state energy per site $E_0/(NJ_1)$ and the staggered magnetization M , for $J_2/J_1 = 0.5, 1, 2$ (for naive Ising expansion) 5, 10, 20 (for modified Ising expansion) and $t = 0$. Nonzero coefficients x^i up to order $i = 10$ for naive Ising expansion or to order $i = 6$ for modified Ising expansion are listed.

i	$E_0/(J_1 N)$			M		
	Naive Ising expansion					
	$J_2/J_1 = 0.5$	$J_2/J_1 = 1$	$J_2/J_1 = 2$	$J_2/J_1 = 0.5$	$J_2/J_1 = 1$	$J_2/J_1 = 2$
0	$-3.33333333 \times 10^{-1}$	$-4.16666667 \times 10^{-1}$	$-5.83333333 \times 10^{-1}$	$5.00000000 \times 10^{-1}$	$5.00000000 \times 10^{-1}$	$5.00000000 \times 10^{-1}$
2	$-1.46708683 \times 10^{-1}$	$-1.53703704 \times 10^{-1}$	$-2.23809524 \times 10^{-1}$	$-7.98687122 \times 10^{-2}$	$-7.14609053 \times 10^{-2}$	$-8.68027211 \times 10^{-2}$
4	$1.10044693 \times 10^{-3}$	$5.08576750 \times 10^{-4}$	$1.36582616 \times 10^{-3}$	$-6.95556119 \times 10^{-3}$	$-5.95673893 \times 10^{-3}$	$-8.37837732 \times 10^{-3}$
6	$-1.39063516 \times 10^{-3}$	$-1.97000255 \times 10^{-3}$	$-2.95007447 \times 10^{-3}$	$-4.80430415 \times 10^{-3}$	$-5.53318319 \times 10^{-3}$	$-7.46816918 \times 10^{-3}$
8	$-5.11831870 \times 10^{-4}$	$-6.87771224 \times 10^{-4}$	$-1.22506627 \times 10^{-3}$	$-3.03361100 \times 10^{-3}$	$-3.35287068 \times 10^{-3}$	$-5.27035727 \times 10^{-3}$
10	$-2.75677029 \times 10^{-4}$	$-4.09491760 \times 10^{-4}$	$-6.02299585 \times 10^{-4}$	$-2.01622805 \times 10^{-3}$	$-2.42979325 \times 10^{-3}$	$-3.42232873 \times 10^{-3}$
	Modified Ising expansion					
	$J_2/J_1 = 5$	$J_2/J_1 = 10$	$J_2/J_1 = 20$	$J_2/J_1 = 5$	$J_2/J_1 = 10$	$J_2/J_1 = 20$
0	-1.83333333	-3.50000000	-6.83333333	$2.77777778 \times 10^{-1}$	$2.77777778 \times 10^{-1}$	$2.77777778 \times 10^{-1}$
1	0.00000000	0.00000000	0.00000000	$6.97167756 \times 10^{-2}$	$3.70370370 \times 10^{-2}$	$1.91158901 \times 10^{-2}$
2	$-1.21179736 \times 10^{-1}$	$-9.07296550 \times 10^{-2}$	$-7.38090200 \times 10^{-2}$	$-4.36538214 \times 10^{-2}$	$-5.67336122 \times 10^{-2}$	$-6.04157972 \times 10^{-2}$
3	$-1.41804384 \times 10^{-2}$	$-3.48154003 \times 10^{-3}$	$-6.42216094 \times 10^{-4}$	$-1.35350826 \times 10^{-2}$	$-7.15990062 \times 10^{-3}$	$-3.64767685 \times 10^{-3}$
4	$4.43598485 \times 10^{-3}$	$3.25869698 \times 10^{-3}$	$1.90188695 \times 10^{-3}$	$-5.47105059 \times 10^{-3}$	$-4.79712404 \times 10^{-3}$	$-6.78984443 \times 10^{-3}$
5	$5.30206875 \times 10^{-3}$	$1.33866469 \times 10^{-3}$	$3.36884895 \times 10^{-4}$	$9.81694291 \times 10^{-3}$	$2.83116612 \times 10^{-3}$	$5.48197309 \times 10^{-4}$
6	$-1.30627826 \times 10^{-3}$	$-1.28650672 \times 10^{-3}$	$-8.82824083 \times 10^{-4}$	$-3.28072052 \times 10^{-3}$	$-5.39705234 \times 10^{-3}$	$-5.29473180 \times 10^{-3}$

TABLE III. Series coefficients for expansions about interlayer coupling of the ground-state energy per site $E_0/(NJ_2)$, the (π, π) gap m/J_2 , and the antiferromagnet susceptibility χ for 4 and 6 layer systems. Nonzero coefficients $(J_1/J_2)^i$ up to maximum order carried out are listed.

i	4 layers			6 layers		
	$E_0/(NJ_2)$	m/J_2	χ	$E_0/(NJ_2)$	m/J_2	χ
0	$-4.040063509 \times 10^{-1}$	$6.589186226 \times 10^{-1}$	1.699358737	$-4.155961890 \times 10^{-1}$	$4.915817770 \times 10^{-1}$	2.403792997
1	0.000000000	-2.149829914	1.161082473×10^1	0.000000000	-2.222865048	2.332835586×10^1
2	$-4.415865088 \times 10^{-1}$	$-9.251531400 \times 10^{-1}$	6.622899086×10^1	$-4.924510549 \times 10^{-1}$	-1.864039733	1.902981798×10^2
3	$-2.554087280 \times 10^{-1}$	-6.521784931	3.610950193×10^2	$-3.192744899 \times 10^{-1}$	-1.517689040×10^1	1.492331708×10^3
4	$-5.884519404 \times 10^{-1}$	-8.897766802	1.876359629×10^3	-1.446337784	-2.769539610×10^1	
5	$-9.377312694 \times 10^{-2}$	-2.575353400×10^1	9.557326563×10^3	$-7.523886385 \times 10^{-1}$	-1.455619317×10^2	
6	-1.120389803	-4.663997073×10^1				
7	$4.729204915 \times 10^{-1}$	-3.236835733×10^2				















